Large nonzero-moment magnetic strings in antiferromagnetic crystals of the manganite type

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The magnetic strings in antiferromagnetic crystals with the spin $S = 1/2$ differ from the magnetic polarons (ferrons) by the absence of the additional magnetic moment. We show that in the $S > 1/2$ double exchange crystals with the antiferromagnetic $s - d$ exchange, a new type of magnetic strings appears which possesses a magnetic moment. It is concentrated at the center of the string, and the magnetized string is, in its essence, the state intermediate between the string and the ferron. In antiferromagnetic manganites, this moment is by an order of magnitude larger than that of a magnetic atom. Unlike the conventional ferrons, the magnetization of the strings exists at any parameters of the crystals under consideration. We argue that this new type of magnetic state can be relevant to some doped antiferromagnets including manganites.

I. INTRODUCTION

The aim of the present paper[*] is to develop a theory of self-trapped charge carrier states for the antiferromagnetic semiconductors of the manganite type, including manganites themselves. They are characterized by the double exchange and by the antiferromagnetic exchange of localized spins with the magnitude S exceeding $1/2$. In contrast to previous treatments, we consider here the situation where the exchange between localized and itinerant electrons is antiferromagnetic, or rather when they have to be antiparallel due to the Pauli principle.

As is well known, a background antiferromagnetic ordering does not ensure the minimum energy of charge carriers. That is why the charge carriers tend to destroy the antiferromagnetic ordering and replace it by another ordering or by a disordered state, at least in their vicinity. The destruction can be either static or dynamic (we neglect the translational motion of ferrons or magnetic strings discussed below, as their bandwidths are very small and the Anderson localization should take place in real crystals).

The tendency toward the static local destruction of an antiferromagnetic order manifests itself in the formation of the magnetic polarons (ferrons) when a free charge carrier becomes self-trapped by a ferromagnetic microregion permanently existing inside an antiferromagnetic host [1,2]. Hence their main feature is an excess magnetic moment as compared with the moment of the electron generating the ferron state.

In principle, the ferrons are possible for the systems without the double exchange independently of the sign of the $s - d$ exchange integral, and in the double exchange systems with the ferromagnetic $s - d$ exchange. (To shorten notation, we speak below about s- and d-electrons, meaning by s the mobile electrons, and by d - the localized ones. In reality the mobile ("s") elecrons may also originate from the same d-shell. Thus, for example, in manganites they are the e_g-electrons or holes, whereas our "d"-electrons are the t_{2g} ones). The conditions for the existence of free ferrons are rather stringent even at $T = 0$. For example, the Néel point T_N should be not very high. But there are also bound ferrons which correspond to an electron trapped by the donor impurities. As discussed e.g. in [2,3], for them the excess magnetization is nonzero for any Néel point though it decreases with increasing T_N. If a region with the complete ferromagnetic ordering is impossible, then a canted antiferromagnetic ordering arises close to the impurity [3,4] (see also references to papers of other authors in review article [3]).

The tendency toward the dynamic destruction of antiferromagnetic order manifests itself in the formation of magnetic strings (in the pioneering paper [5] they were called quasioscillators). Strings are traces of wrong spins left on the trajectory of an extra electron or hole when it moves in an antiferromagnetic background in a situation described by the nondegenerate Hubbard model. In this state, a charge carrier moves by interchanging with the neighboring spins, so that as a result the net magnetization does not change, remaining essentially zero. (The formation of such strings and the resulting electron or hole confinement was rediscovered [6,7] much later than the first paper [5] appeared, after the interest to such model was raised by the discovery of high-temperature superconductivity).

For this quasiparticle, oscillations of the magnetic disorder are accompanied by the oscillations of the electron density. This disordering excludes the possibility of the

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free charge carrier motion, and hence the standard scenario of the ferron formation is impossible here. The existing theory of the strings [5–7] is related to the systems described by the Hubbard Hamiltonian that are equivalent to double-exchange systems with the magnetic atom of spin $S = 1/2$ and the negative (antiferromagnetic) sign of the $s - d$ exchange integral, which ensures the zero total spin of an atom occupied by an s-electron [2]. As explained above, unlike ferron, the magnetic string with $S = 1/2$ does not possess an additional magnetic moment as compared with the moment of the self-trapped electron.

Meanwhile, the case of spins S exceeding $1/2$ is important for real materials, but was not investigated yet. It can be described by the $s - d$ model with the antiferromagnetic on-site $s - d$ exchange. The free motion of the charge carriers is again impossible in this case, and the strings arise, see Fig.1 below. However, as we will show, the strings in such systems differ from the strings in a $S = 1/2$ magnetic system since they can have an excess magnetic moment. This moment will be concentrated in a region around the equilibrium point, i.e. the core. The central part of this object can be ferromagnetic (ferromagnetic polaron, or ferron), whereas the motion of charge carriers outside this core region occurs in a string-like fashion. Thus, the resulting state may be visualized as a combination of the inner ferron [1] and outer string [5] regions.

As will be shown below, the string excess moment exists for arbitrary parameters of the system under consideration. In the crystals with sufficiently low Néel temperatures T_N, a microregion with the complete ferromagnetic ordering should exist. Hence such a state may be interpreted as a mixed string-ferron state. But for the crystals with sufficiently high T_N, the complete ferromagnetic ordering should be replaced by the canted antiferromagnetic one (the canted ordering arises since the antiferromagnetic superexchange in the high-T_N systems is too strong to be completely suppressed by the ferromagnetic indirect exchange via the bound charge carrier). The existence of the excess magnetic moment at any T_N stems from the fact that the string state is a bound state resembling the state of an electron trapped by a donor. The fact that the force in the former case is quasielastic and not the Coulomb is nonessential, as both these forces cause the electron confinement. In other words, the electron localization for the magnetized string is caused not by the arising magnetized region but by the quasielastic force.

The calculations carried out below show, in particular, that such quasiparticles should exist in manganites [3,8,9] when they are antiferromagnetic, and their magnetic moment should be an order of magnitude larger than the moment of a separate Mn^{3+} ion. (Strictly speaking, our treatment will be carried out for the slightly doped simple two-sublattice antiferromagnet with the G-type struc-

ture, whereas undoped $LaMnO_3$ has the layered A-type structure. But the general physical mechanism, considered in this paper, should work in this case as well, albeit with some modifications; besides, there exist many other magnetic systems with the G-type structure which can be doped and which could be described by our model.)

The mobility of the magnetized strings, like that of the conventional ferrons, is too low to affect the conductivity. However, they can produce a significant effect on magnetic properties of the system. As is well known, the existence of the "ready at hand" large magnetic moments in an antiferromagnetic semiconductor leads to a steep rise in the magnetization under a weak external magnetic field. This effect is often observed experimentally. Certainly, in a nondegenerate semiconductor all these quasiparticles are bound to the donor (acceptor) impurities at $T \to 0$. But, at finite temperatures, the ferrons can become free, i.e. become located far from impurities. Just these ferrons contribute to the jump in the magnetization. For this reason, the evaluation of their moments is important for the interpretation of the experimental data.

II. MODEL

The problem of the energy spectrum in the double exchange systems is treated using the $s-d$-model as a basis:

$$H_{sd} = -t \sum a^*_{\mathbf{g}\sigma} a_{\mathbf{g}+\mathbf{\Delta}\sigma} - A \sum (\mathbf{s}\mathbf{S_g})_{\sigma\sigma'} a^*_{\mathbf{g}\sigma} a_{\mathbf{g}\sigma'}$$

$$-\frac{I}{2} \sum \mathbf{S_g}\mathbf{S_{g+\Delta}}, \qquad (1)$$

where $a^*_{\mathbf{g}\sigma}, a_{\mathbf{g}\sigma}$ are the s-electron operators corresponding to the conduction electrons or holes at atom $\mathbf{g}$ with spin projection σ, $\mathbf{s}$ is the s-electron spin operator, $\mathbf{S_g}$ that of the d-spin of atom $\mathbf{g}$, $\mathbf{\Delta}$ is the vector connecting the first nearest neighbors. The crystal structure is assumed to be simple cubic. As usually, the inequality $t \gg |I|S^2$ must be met as the hopping integral t is of the first order of magnitude, and the $d - d$ exchange integral I of the second order in the small d- orbit overlapping (I should be negative to ensure the antiferromagnetic ordering).

In what follows, the condition of the double exchange $12t \ll |A|S$ will be assumed to be met, with the $s - d$ exchange integral A being negative. Under these conditions, in the zero approximation in W/AS ($W = 12t$) , the charge carrier is fixed at one of the magnetic atoms, their total spin being $S - 1/2$.

It is necessary to establish first when model (1) with $A < 0$ is realistic. To begin with, in reality, the double exchange takes place when a charge carrier is an extra or deficient electron in the d-shell of transition metal compounds. According to the Hund rule, the $d - d$ exchange

is ferromagnetic; the same should be true for the exchange between the conduction electron and the rest of the d-spins, which form the localized spins of the magnetic atoms. According to the Pauli principle, the total spin of the atom, occupied by a conduction electron at a certain moment of time, cannot exceed $5/2$. Hence the charge carrier spin is parallel to the total spin of the other atoms only for $S \leq 2$.

If $S \geq 5/2$, despite the ferromagnetic on-site exchange, the spin of the charge carrier is antiparallel to the total spin of the rest of the d-electrons. Hence in this case an antiferromagnetic $s-d$ exchange integral should be chosen in the $s-d$ model. The same should be done, if the charge carrier is a hole, and $S \leq 5/2$. Really, if the $s-d$ Hamiltonian (1) is written in terms of the hole operators, the energy of the hole is opposite in sign to the corresponding electron energy. Thus, the assumption of an negative A is justified for S not less than $5/2$ or not larger than $5/2$ if the charge carriers are the electrons or the holes, respectively. In particular, the latter condition is met for the manganites with the hole conductivity and $S = 2$ for the Mn^{3+} ions.

It should be noted that in the case of the electrons the negative A looses the meaning of the Hund's exchange integral and reflects only the Pauli principle. But this is nonessential, as quantity A enters only in the zeroth approximation in W/AS via an additive constant $A(S+1)/2$, which can be omitted. The point is that the quantity A does not enter the terms of the first approximation in the effective Hamiltonian (2) which describe the double exchange.

This consideration can be readily generalized to the case when the crystal field splits the d-level so strongly that the gap between the sublevels exceeds the $s-d$ exchange energy, and all the d-electrons occupy states inside the lowest sublevel. Then the value of the maximum spin of the entire d-shell should be replaced by that of the lowest d-sublevel when considering the problem in a way similar to that just used. If the lowest sublevel is completely filled, the role of the entire d-shell is played by the upper level.

As mentioned in the Introduction, to simplify the treatment, the magnetic ordering is assumed to be staggered instead of the layered one which is realized in the undoped manganites. Conventional strings in layered antiferromagnetic structures with $S = 1/2$ were considered in Ref. [9]. It should be pointed out that for $A > 0$ the charge carrier motion is band-like though at the antiferromagnetic ordering the band is considerably narrower than for the ferromagnetic that. Conventional ferron states are possible in this case [1,2].

III. NONMAGNETIZED MAGNETIC STRINGS

Before carrying out real calculations, we first explain qualitatively the origin and the nature of the string states in our case. Consider an antiferromagnet with the localized spins S forming a simple two-sublattice Néel structure, and let us put an extra electron at site a with the spin $S^z = S$. In the situation considered (e.g. $S = 5/2$), it would necessarily have spin down — or, more accurately, the total spin of this state will be $S - 1/2$. In our model, only this extra electron ("s"-electron) can move to a neighboring site. But if we consider the resulting situation classically, this extra electron with spin down will not be able to move at all, because at the neighboring sites there already exists spins down (e.g. $S^z = 5/2$), so that the Pauli principle forbids such motion.
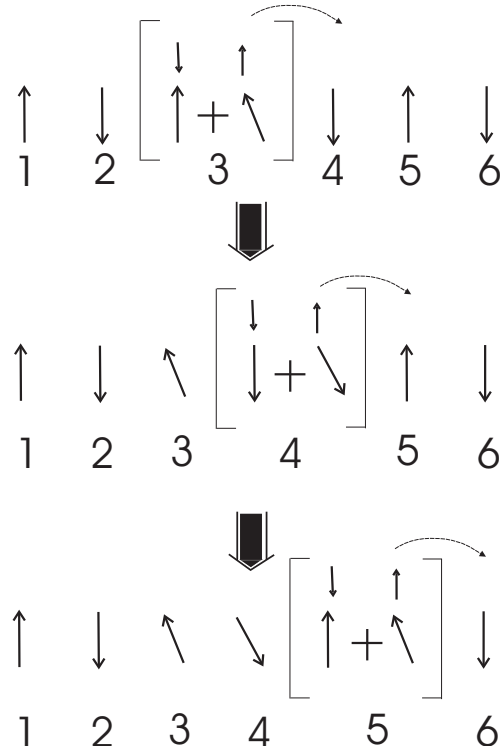

FIG. 1. Schematic picture explaining the formation of a string (deviations of the localized spins (large arrows)) in the process of motion of the conduction electron (small arrow). The exchange interaction of these tilted spins with the surrounding antiferromagnetic spins in two- and three-dimensional cases (not shown) will lead to an energy increase proportional to the length of the electron trajectory.

However the situation changes if one takes into account the quantum nature of spins. The state with the total spin $S_{tot} = S - 1/2$ at an initial site a is not necessarily that with the localized spin $S^z = S$ and the spin of the s-electron $s^z = -1/2$: it also has another component, with the localized spin $S^z = S - 1$, and $s^z = +1/2$,

$$|S_{tot} = (S-1), S_{tot}^z = (S-1)\rangle$$

$$= \alpha\,|S^z = S, s^z = -1/2\rangle + \beta\,|S^z = (S-1), s^z = 1/2\rangle$$

The s-electron can hop to a neighboring site b owing to the second part of this wave function. But then there will be a spin deviation left at the initial site a: instead of the state with $S^z = S$, as in the beginning, now it will have $S^z = S - 1$. This process can be repeated, and as a result the charge carrier will move, but leaving the trace of spin deviations left at its trajectory. This is illustrated in Fig.1.

As we see, this process is quite similar to the one, which leads to a string formation in a nondegenerate Hubbard model [5], see also [10]. The difference is that in this case, it is not a completely reversed spin which will be left on a trajectory of a charge carrier, but the spin deviation of a large spin S. But, similar to the case of [5], one immediately sees that the trace of wrong spins would cost us an energy of the exchange interaction with the neighbors (in two- and three-dimensional systems) proportional to the length of the trajectory, which would finally lead to a confinement of the electron (if one ignores the spin-flip processes and the Trugman trajectories [11], which give only a small contribution in the case of large spin S). However, in addition to that, we will show that the string formation in this case can be accompanied also by the formation of the magnetized "core", so that the resulting object would have a nonzero magnetic moment.

We go now to the mathematical treatment of this problem. First, we consider the case when the magnetic moment of the string is negligibly small. We use the special version of the perturbation theory in W/AS developed in Refs. [2,12]. It makes possible to construct an effective electron-magnetic Hamiltonian H_{ef} for the system under consideration, in which the d-spins are considered as quantum operators. This Hamiltonian is exact to the first order in AS/W, and no additional approximations (mean field etc.) are used.

To construct the Hamiltonian, an effective spin of magnitude S is ascribed to each magnetic atom, independently of its being empty or occupied by an s-electron. In the last case, it formally increases the number of spin degrees of freedom by 1 as compared with their initial real number. But the structure of the effective Hamiltonian ensures vanishing of the contribution from the extra degree of freedom. As for the charge carriers, they are treated as spinless fermions with operators $c_{\mathbf{g}}^*, c_{\mathbf{g}}$. This Hamiltonian has the form

$$H_{ef} = \frac{A(S+1)}{2}\sum c_{\mathbf{g}}^* c_{\mathbf{g}} - t\sum F(\mathbf{S_g}, \mathbf{S_{g+\Delta}})c_{\mathbf{g}}^* c_{\mathbf{g+\Delta}} -$$

$$-\frac{I}{2}\sum \mathbf{S_g S_{g+\Delta}}, \qquad (2)$$

with $\quad (2S+1)F(\mathbf{S_g}, \mathbf{S_{g+\Delta}}) =$

$$\sqrt{(S + S_{\mathbf{g}}^z)(S + S_{\mathbf{g+\Delta}}^z)} + \frac{1}{\sqrt{S + S_{\mathbf{g}}^z}} S_{\mathbf{g}}^+ S_{\mathbf{g+\Delta}}^- \frac{1}{\sqrt{S + S_{\mathbf{g+\Delta}}^z}}$$

In Eq.(2) small terms of the order of IS^2/t describing a change in the $d - d$ exchange of the atom bearing the charge carrier are omitted. An explicit expression for them is presented in Refs. [12].

In what follows, the upper and lower bounds for the nonmagnetized string energy will be found which allows to make the string theory more general and more accurate as compared with previous theory for $S = 1/2$. Calculations show that two quite different approaches lead to results which are very close. Hence both these approaches are reliable at the actual values of parameters.

We begin with the carrier located at the central atom $\mathbf{0}$ when the ordering is complete antiferromagnetic. This means that the spin projection of each atom is maximum in the local coordinate system, in which the z-axis coincides with the moment of the sublattice of this atom. As is seen from Eq. (2), only such hole transitions to the neighboring atoms are possible, when at the atom left by the hole, the deviated spin remains with the spin projection $S - 1$ in the local coordinate system. At the next step the second deviated spin arises. and so on. As a result, the motion of the hole along a path beginning with the central atom is accompanied by the deviation of spins from the moments of their sublattices along this path, see Fig. 1.

The wave function of the system is sought in the form, in which the possibility of the d-spin deviations more than by 1 is ignored as their relative weight is small ($\propto 1/z$ where z is the coordination number):

$$\Psi_s = \sum_{i=0, \mathbf{\Delta}_1 \ldots \mathbf{\Delta}_i} X(\mathbf{\Delta}_0, \mathbf{\Delta}_1, . \mathbf{\Delta}_i) c_{\mathbf{\Delta}_0 + \mathbf{\Delta}_1 + \ldots \mathbf{\Delta}_i}^* |0> \times$$

$$\prod_{k=0}^{i-1} \frac{S_{\mathbf{\Delta}_0 + \mathbf{\Delta}_1 + \ldots \mathbf{\Delta}_k}^-}{\sqrt{2S}} \prod_{\mathbf{f}} \delta(S_{\mathbf{f}}^z, S), \qquad \mathbf{\Delta}_0 \equiv \mathbf{0} \qquad (3)$$

written using the relationship (see, e.g., Ref. [2])

$$S^- \delta(S^z, m) = \sqrt{(S+m)(S-m+1)}\,\delta(S^z, m-1).$$

Here $|0>$ is the spinless fermion vacuum wave function, $\delta(S^z, m)$ is the d-spin wave function with the spin projection m equivalent to the Kronecker symbol $\delta_{S^z, m}$. To simplify the form of Ψ_s in Eq. (3), unlike the Hamiltonian (2), the local coordinate system is used for each atom, in which the z axis coincides with the moment of the sublattice to which the spin belongs. When one calculates the matrix elements of Hamiltonian (2) with the use of Ψ (3), one should use the common coordinate system, for example, corresponding to the sublattice I, and

then for the atoms of the sublattice II one should change the sign of the d- spin projection and replace S^- by S^+.

The string wave equation is obtained from Eqs. (2), (3) in the form

$$(E - nL)X(\mathbf{\Delta}_0, \mathbf{\Delta}_1, ...\mathbf{\Delta}_n) =$$

$$= -t_s \sum_{\mathbf{\Delta}_{n+1}} X(\mathbf{\Delta}_0, \mathbf{\Delta}_1 ..\mathbf{\Delta}_n, \mathbf{\Delta}_{n+1}), \qquad (4)$$

$$t_s = \frac{t\sqrt{2S}}{2S+1}, \qquad L = |I|S(z-2)$$

where L is the change in the $d-d$ exchange energy due to the spin deviation. Strictly speaking, this expression is valid for $n > 1$ if the paths are not self-crossing and self-contacting but the number of such paths is very small (just they lead to the motion of the string center over the crystal [13]). The same equation can be obtained by a direct expansion of the wave function Ψ_s in the eigenfunctions of the second term of the Hamiltonian (1).

To solve Eq. (4), an effective wave function is introduced for the string by summing over the paths, which lead to the same point:

$$\phi(\mathbf{f}) = \sum_n \phi_n(\mathbf{f}),$$

$$\phi_n(\mathbf{f}) = \sum_{\mathbf{\Delta}_1 ... \mathbf{\Delta}_n} X(\mathbf{\Delta}_0, \mathbf{\Delta}_1, ..\mathbf{\Delta}_n)\delta(\mathbf{\Delta}_1 + ... \mathbf{\Delta}_n, \mathbf{f}), \qquad (5)$$

where $\delta(\mathbf{x}, \mathbf{y})$ is tantamount to the three-dimensional Kronecker symbol.

Multiplying both sides of Eq. (4) by $\delta(\mathbf{\Delta}_1 + ... \mathbf{\Delta}_n, \mathbf{f})$ and summing over all $\mathbf{\Delta_i}$ and n, one obtains:

$$\left[L \sum_n n\phi_n(\mathbf{f}) - E_s\phi(\mathbf{f}) \right] = t_s \sum_{\mathbf{\Delta}} \phi(\mathbf{f} + \mathbf{\Delta}). \qquad (6)$$

To obtain the lower bound for the string energy, one should assume that the hole reaches the atom $\mathbf{f}$ using the shortest way, i.e. one sets

$$\sum_n n\phi_n(\mathbf{f}) = f\phi(\mathbf{f}) \qquad (7)$$

(for the one-dimensional case this equation is exact).

The effective mass approximation is used. For the spherically symmetric potentials the ground state wave function is given by [14]

$$\phi(r) = \frac{\chi(r)}{r}, \qquad \chi(0) = 0 \qquad (8)$$

As a consequence of Eqs (7), (8), one arrives at the wave equation for the wave function χ_l corresponding to the lower bound:

$$\left(-\frac{1}{2m_s}\frac{d^2}{dr^2} + \frac{L}{a}r - 6t_s - E_s^l \right)\chi_l(r) = 0, \qquad (9)$$

where $\hbar = 1$, a is the lattice constant, $z = 6$ is the coordination number, $m_s = 1/(2t_sa^2)$ is the effective mass of the hole bound to the fixed center of the string state and has nothing in common with the motion of the quasiparticle over the crystal.

Eq. (9) can be solved exactly, cf. [5]. The ground state is described by the wave function

$$\phi_l(r) = \frac{Ai[r/\rho - a(E_s^l + 6t_s)/\rho L]}{r},$$

$$\rho = (a/2m_sL)^{1/3} = a(t_s/L)^{1/3}, \qquad (10)$$

where $Ai(r)$ is the Airy function, ρ is the string radius. According to Eq. (8) the energy should be found using the maximum negative value of zeroes of the Airy function presented in Ref. [15]. Then one obtains the lower bound for the string energy:

$$E_s^l = -6t_s + 2.3L^{2/3}t_s^{1/3}. \qquad (11)$$

This result is again similar to a nondegenerate case $(S = 1/2)$ [5]. For the typical values of the manganite parameters t_s about 0.1 eV (the initial band width $2zt_f = 1.2$ eV, $S = 2$) and L about 0.01 eV the string radius ρ amounts to about 2 lattice constants, and E_s^l = - 0.35 eV (this energy is counted from the band center). As is seen from this estimate, the lower bound for the string energy is rather close to the band bottom of a particle with the bandwidth $2zt_s$.

To obtain the upper bound for the string energy, it is sufficient to assume that the hole reaches the atom $\mathbf{f}$ by random walks. Then for n sufficiently large the probability to reach the site $\mathbf{f}$ after n steps is [16]

$$p_n(\mathbf{f}) = \frac{1}{(2\pi n)^{3/2}}\exp\left(-\frac{f^2}{2n}\right). \qquad (12)$$

One obtains the following values for the averaged values of f and f^2 from Eq. (12): $< f >= 1.596\sqrt{n}, < f^2 >= 3n$. Hence, the dispersion is sufficiently small, and to find the upper bound for the string energy E_s^u, one should solve the following wave equation:

$$\left(-\frac{1}{2m_s}\frac{d^2}{dr^2} + \frac{L}{2.5a^2}r^2 - 6t_s - E_s^u \right)\chi_u(r) = 0. \qquad (13)$$

The solutions of Eq. (13) with the boundary condition (8) are the wave functions of an one-dimensional oscillator with uneven quantum numbers. Hence the ground-state value of this number is 1, and the zero-point energy

of a three-dimensional oscillator is not $\omega/2$ but $3\omega/2$. This yields:

$$E_s^u = -6t_s + 1.9(t_s L)^{1/2}. \qquad (14)$$

For the parameters used above, $E_s^u = -5.2t_s$. The fact that E_s^u and E_s^l presented above virtually coincide is a consequence of the fact that, strictly speaking, Eq. (13) is valid for very large f, i.e., for small L/t_s, and its value adopted here is not very small. If one takes the L value an order of magnitude less, then E_s^u exceeds E_s^l by 0.1 t_s. In any case, the approach based on (7) ensures a reasonable accuracy at actual parameter values. The reason for it is the fact that longer paths to the same point correspond to larger energies of the magnetic disordering, and hence their weight is small as compared with the shortest path. The approach based on (7) will be used for investigation of the magnetized strings in the next Section.

IV. MAGNETIZED MAGNETIC STRINGS

Keeping in mind that according to Eq. (4) $t_s \propto (2S)^{-1/2}$, one sees that the string state disappears in the classical limit $S \to \infty$. Hence, in this case, the only way to allow at least for some motion of an electron to decrease its kinetic energy, would be by creating the ferron state. But we can combine both these possibilities by making a ferromagnetic microregion in the centre of the string. Consequently, we should treat two problems: the motion of an electron inside a ferromagnetic microregion of radius R (to be determined by the minimization of the total energy), and the string-like motion outside this region. The solutions should be matched at the boundary of the ferron.

As is seen from Eq. (2), the effective hopping integral for the ferromagnetic ordering is

$$t_f = \frac{2St}{2S+1},$$

i.e., exceeds t_s by a factor of $\sqrt{2S}$. Hence, the ferromagnetic region is a potential well for the carrier of a depth

$$U = z(t_f - t_s) = z\frac{2St}{2S+1}\left(1 - \frac{1}{\sqrt{2S}}\right) \qquad .(15)$$

As follows from Eq. (15), the string magnetization is possible only for $S > 1/2$.

The state of the charge carrier inside the spherical potential well of a radius R with a ferromagnetic ordering is found from the equation

$$-t_f(z + a^2\Delta)\psi = E_{ms}\psi \qquad (r < R) \qquad (16)$$

where E_{ms} is the magnetized string energy. As for the antiferromagnetic region outside the sphere of the radius R, the same approximation as in Eq (9) will be made:

$$[-t_s(z+a^2\Delta)+\frac{L}{a}(r-R)]\psi = E_{ms}\psi, \qquad (r > R). \qquad (17)$$

The ground-state solutions of Eqs (16) and (17) are, respectively (Eq (8) is used):

$$\chi = \sin pr, \qquad tp^2a^2 = (E_{ms}+zt_f), \qquad (r < R) \qquad (18)$$

$$\chi = Ai(-\xi),$$

$$\xi = \left(-\frac{r-R}{a} - \frac{U}{L} + \frac{p^2a^2t_f}{L}\right)\left(\frac{L}{t_s}\right)^{1/3}. \qquad (19)$$

An equation (boundary condition) describing the matching of the wave functions outside and inside the ferromagnetic region has the form

$$ap\cot(pR) = \frac{L^{1/3}}{t_s^{1/3}}\frac{dAi(-\xi)/dr|_{r=R}}{Ai(-\xi)|_{r=R}}. \qquad (20)$$

To calculate the right-hand side of Eq. (20), the asymptotic expression for $Ai(-\xi)$ will be used, which is valid at $\xi \to -\infty$:

$$Ai(-\xi) = \frac{1}{2|\xi|^{1/4}}\exp\left(-\frac{2|\xi|^{3/2}}{3}\right). \qquad (21)$$

Formally this expression is valid for $\xi \gg 1$ but practically is sufficiently accurate beginning with $\xi = 1$ [15]. Then one can rewrite Eq. (20) in the form

$$ap\cot(pR) = -(2S)^{1/4}(V-a^2p^2)^{1/2}, \qquad V = \frac{U}{t_f}. \qquad (22)$$

Eq. (22) makes it possible to find p as a function of R and then to find the R value which gives the minimum of the total energy of the system:

$$E_{ms} = -6t_f + p^2a^2t_f + \frac{4\pi R^3 D}{3a^3},$$

$$D = z|I|S^2 = \frac{3LS}{2}, \qquad (23)$$

where D is the $d-d$ exchange energy spent for formation of the ferromagnetic microregion (per atom). Technically, it is more convenient to fix a p value and to find the lowest R value for which the Eq. (22) is met.

Numerical calculations were carried out for $S = 2$. In the range of R/a values between 4.81 and 1.08, the solutions of Eq. (22) can be presented approximately in the form

$$ap(R) = \frac{3.4}{0.9 + R/a}. \qquad (24)$$

As should be the case, keeping in mind that 3.4 is sufficiently close to π, one arrives at the same expression for $R \gg a$ as for the ferron energy found in Refs. [1,2]. But

quite different is the case of R comparable to a. Then the condition for the magnetized string existence differs from that for the ferron existence drastically.

The minimization of the energy (23), (24) with respect to R yields an expression for the energy of the $d - d$ exchange D as a function of $x = R/a$:

$$\frac{D(x)}{t_f} = \frac{1.84}{(0.9 + x)^3 x^2}. \qquad (25)$$

It shows that a completely ferromagnetic region arises when $D/t_f < 0.27$. Then $R = a$, and the magnetized string energy (23) is lower than the string energy (9) though the difference is small. Energy E_{ms} decreases and the size R of the ferromagnetic region increases with diminishing ratio D/t_f. For example, for $D/t_f = 0.01$ energy E_{ms} is - 3.45 t_f = - 6.9t_s and the radius R is about $2a$. This magnetized string energy is lower than the lower bound for the nonmagnetized string energy (9) equal to -5.83 t_s.

Numerical estimates for the manganites can be obtained using the well-known mean field expression for the Néel point $T_N = D(S+1)/3S$, its experimental value 140 K and t_f is about 0.1 eV. Then one obtains R close to a. This means that a free string-ferron has a magnetic moment close to zS. In other words, it should be an order of magnitude larger than the moment of a Mn^{3+} ion. If ratio D/t_f is larger than 0.27, formally R is less than a; this means that the magnetized region is rather a canted antiferromagnetic, and not a ferromagnetic one. The situation resembles that for the bound ferrons [3,4]. But it seems not very actual.

V. CONCLUSIONS

Summarizing, we considered in this paper the motion of charge carriers in doped antiferromagnets in case when the localized electrons have total spin $S > 1/2$ and, due to the Pauli principle, spins of doped electrons or holes are opposite to the localized spins (i.e. when the total spin on a site with an extra electron or hole is $S - 1/2$). We have shown that the motion of charge carriers in this case is possible by forming strings — traces of spin deviations. Such string states by themselves would not have any extra magnetization. However the better state, with lower energy, may be created in this case: the central part of this state will be a ferromagnetic polaron (ferron) or a strongly canted region, and the motion of an electron outside this region proceeds in a string-like fashion. Thus, this state combines the features of both the ferron states [1] and of the string states [5]. The extra magnetic moment, associated with each charge carrier in this case, could significantly modify magnetic properties of such systems. We believe that the physics described above may be relevant for the low-doped manganites; there may be also other materials belonging to this class.

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